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COSMO-RS based prediction for alpha-linolenic acid (ALA) extraction from microalgae biomass using room temperature ionic liquids (RTILS) (Article)

(Open Access)

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Abstract

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One of the essential fatty acids with therapeutic impacts on human health is known to be omega-3 polyunsaturated fatty acids (PUFA). More lately, ionic liquids (ILs) have received significant attention among scientists in overcoming the disadvantages of traditional solvents in biomass lipid extraction. However, the large pool of cations and anions possibly accessible will lead to a growing number of innovatively synthesized ILs. Nevertheless, the exhaustive measurement of all these systems is economically impractical. The conductive screening model for real solvents (COSMO-RS) is considered a precious approach with the availability of a few models to predict the characteristics of ILs. This work introduces the estimate of capacity values at infinite dilution for a range of ILs using COSMO-RS software as part of solid-liquid extraction. This favorable outcome presented that the capacity values of the IL molecules are extremely dependent on both anions and cations. Among the 352 combinations of cation/anion tested, short alkyl chain cations coupled with inorganic anions were found to be most efficient and therefore superior in the extraction method. Sulphate-, chloride-, and bromide- based ILs were found to have higher extraction capacities in contrast with the remainders, while propanoate revealed an extraordinary capacity when combined with ethyl- based cations. Eventually, the predicted results from COSMO-RS were validated through the experimentally calculated extraction yield of alpha-linolenic acid (ALA) compound from Nannochloropsis sp. microalgae. Three selected ILs namely [EMIM][Cl], [TMAm][Cl], and [EMPyrro][Br] were selected from COSMO-RS for empirical extraction purpose and the validation results pinpointed the good prediction capability of COSMO-RS. © 2020 by the authors.

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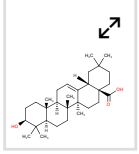
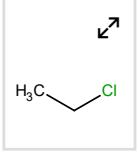
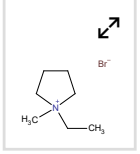
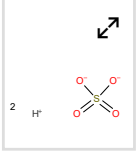
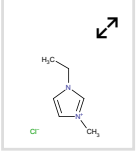
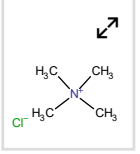

Author keywords

ALA extraction | Capacity at infinite dilution | COSMO-RS | Ionic liquids | Omega-3 PUFAs | Solid-liquid extraction | Tetramethyl ammonium

Indexed keywords

EMTREE drug terms: bromide | chloride | ionic liquid | linolenic acid | sulfate | anion | cation | ion | ionic liquid | linolenic acid

EMTREE medical terms: Article | biomass | dilution | extraction | microalga | nonhuman | prediction | room temperature | software | validation process | chemical structure | chemistry | molecular model | temperature | thermodynamics

MeSH: alpha-Linolenic Acid | Anions | Cations | Computational Chemistry | Ionic Liquids | Ions | Microalgae | Models, Molecular | Molecular Structure | Temperature | Thermodynamics

Chemicals and CAS Registry Numbers:

bromide, 24959-67-9; chloride, 16887-00-6; linolenic acid, 1955-33-5, 463-40-1; sulfate, 14808-79-8;

alpha-Linolenic Acid; Anions; Cations; Ionic Liquids; Ions

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Funding text #2

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